

Topological Insulator in the Presence of Spatially Correlated Disorder

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We investigate the effect of spatially correlated disorder on two-dimensional topological insulators and on the quantum spin Hall effect which the helical edge states in these systems give rise to. Our work expands the scope of previous investigations which found that uncorrelated disorder can induce a non-trivial phase called the topological Anderson insulator (TAI). In extension of these studies, we find that spatial correlations in the disorder can entirely suppress the emergence of the TAI phase. We explain this phenomenon by generalizing an existing effective medium theory to the case of correlated disorder potentials. The predictions of this theory are in good agreement with our numerics and may be crucial for future experiments.

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I. INTRODUCTION

A two-dimensional topological insulator¹ features edge states similar to those of the quantum Hall effect with the difference that electrons of different spin move in the same direction at opposite edges. Accordingly, this so-called “quantum spin Hall effect” (QSHE)² can be understood as two non-interacting copies of a quantum Hall system, one for each spin. The stability of the edge states is guaranteed by time-reversal symmetry which forbids scattering into the counter-propagating edge state with opposite spin.^{3,4} These properties, which have recently attracted considerable attention,^{5–10} make topological insulators promising candidates for key components in future spin-tronic devices^{11,12}. In 2006 HgTe/CdTe quantum wells were proposed as suitable systems for a first experimental realization of the QSHE¹³ which was, indeed, achieved shortly thereafter.^{14,15} Numerically it was found that the edge states in a topological insulator not only show great robustness against disorder but also that strong disorder itself can induce a phase featuring pure edge transport even if the system is an ordinary insulator in the clean limit.¹⁶ This disorder-induced and topologically non-trivial phase was named topological Anderson insulator (TAI). In 2009 a theory was put forward¹⁷ that lead to a detailed understanding of the TAI, showing that disorder causes a negative correction to the topological mass which pushes the system into the TAI phase. This interesting phenomenon has meanwhile been investigated numerically in a variety of different systems^{18–22} including the case of a three-dimensional topological insulator.²³ However, due to the challenges involved in controlling the disorder in a HgTe/CdTe quantum well, the TAI has not yet been realized experimentally. This problem might be overcome by employing ultra-cold atomic gases in optical lattices for the realization of a topological insulator.²⁴ In such a highly tunable model system the disorder could be introduced by an optical laser speckle potential^{25,26} which has the advantage of being under external control.

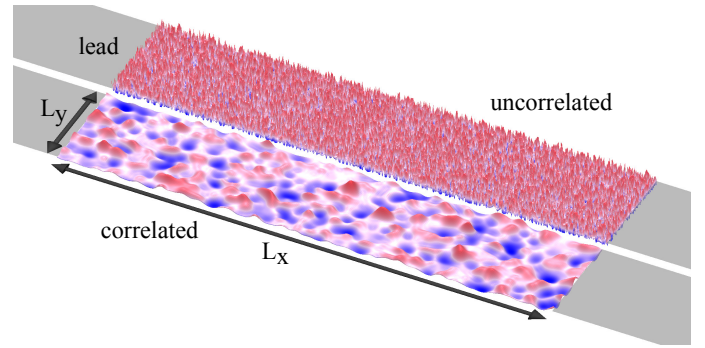


FIG. 1. (color online). Illustration of the scattering setup for the considered topological insulator: a rectangular disordered middle part of height L_y and width L_x is attached to two semi-infinite leads on the left and right. Random potentials with and without correlations between neighboring grid points in the underlying lattice discretization are shown in the bottom and top panel, respectively.

An important point to emphasize in this context is that both the speckle pattern for cold atomic gases as well as the disorder which naturally occurs in a quantum well are characterized by a finite spatial correlation length ξ . Since this correlation has been disregarded in all previous numerical studies of the TAI which we are aware of^{16,17,22,27,28} the question was posed²⁸ how a finite correlation length ξ would influence the predictions for the appearance and for the stability of the TAI. In view of the fact that spatial correlations in the disorder have already been shown to play an important role in the context of various other scattering scenarios^{29–42} one may expect such correlations to be a relevant factor also for topological insulators. We address this topic by studying explicitly how a static and spatially correlated disorder influences the transport characteristics of topological insulators (Fig 1). As we will specify in detail below, our numerical results show marked deviations from conventional simulations with uncorrelated disorder.

II. METHOD

We proceed along the lines of previous studies, where an appropriate description of the two dimensional HgTe/CdTe quantum well was proposed in terms of an effective Hamiltonian.¹³ This Hamiltonian which was derived based on the $\mathbf{k} \cdot \mathbf{p}$ perturbation theory and the six-band Kane-model takes the following form:

$$H_{\text{eff}}(k_x, k_y) = \begin{pmatrix} h(\vec{k}) & 0 \\ 0 & h^*(-\vec{k}) \end{pmatrix}, \quad (1)$$

with

$$\begin{aligned} h(\vec{k}) &= \mathbb{1}\epsilon(\vec{k}) + d_i(\vec{k})\sigma^i \\ \epsilon(\vec{k}) &= C - D(k_x^2 + k_y^2) \\ d_i &= \begin{pmatrix} Ak_x \\ -Ak_y \\ M(\vec{k}) \end{pmatrix} \\ M(\vec{k}) &= m - B(k_x^2 + k_y^2) \end{aligned} \quad (2)$$

and σ^i labelling the Pauli-matrices. The basis of this effective Hamiltonian consists of the s-like E1 and the p-like heavy-hole H1 quantum well sub-bands for spin up (+) and down (-). The ordering is chosen to be $|E1+\rangle, |H1+\rangle, |E1-\rangle, |H1-\rangle$. Since the spin-up and spin-down parts in the Hamiltonian are decoupled as a consequence of time reversal symmetry⁴³ it is sufficient for our calculations to only use the spin-up block $h(\vec{k})$. The solution for the spin-down block follows from a time-reversal operation. The material-dependent constants A , B and D in all our calculations are set to realistic values $A = 364.5 \text{ meV nm}$, $B = -686 \text{ meV nm}^2$, $D = -512 \text{ meV nm}^2$ and $C = 0 \text{ meV}$ taken from Ref. [44]. The sign of the topological mass m has a strong impact on the system's transport behavior: for positive m the system behaves like an ordinary insulator with a band gap of $2|m|$, whereas if m is set to a negative value the system turns into a topological insulator featuring perfectly transmitting edge states for the Fermi energy E_F lying inside the bulk band gap $|E_F| < |m|$. To simulate such a system we use the experimentally determined value⁴⁴ of $m = -10 \text{ meV}$.

The scattering geometry which we consider consists of a rectangular disordered region of width L_x and height L_y attached to two clean, semi-infite and undoped leads (see illustration in Fig. 1). We discretize the scattering region on a square lattice with grid constant a using the tight-binding approximation in the continuum limit for the implementation of the effective Hamiltonian. If not stated otherwise, the grid-constant a is set to 5 nm , in agreement with the value used in previous studies.^{16,17,27,45,46} For simplicity, we consider the limit of vanishing temperature $T \rightarrow 0$ and infinitely small bias voltages $V \rightarrow 0$ applied between the two semi-infinite leads. According to the Landauer-Büttiker formalism the conductance G in this limit is proportional to the transmission probability

T at the Fermi energy E_F ,

$$G = \frac{e^2}{h} T = \frac{e^2}{h} \sum_{n,m}^N |t_{nm}|^2. \quad (3)$$

The indices n and m extend over all N lead modes and t_{nm} labels the transmission amplitude from mode n in the incoming lead to mode m in the outgoing lead. Since we consider both spins separately, every mode only contributes a single conductance quantum e^2/h . For the calculation of the transmission we employ the advanced modular Recursive Green's function method⁴⁷⁻⁴⁹ which incorporates the disorder by way of a static on-site energy-value $V(\vec{x})$ imposed at every grid-point $\vec{x} = (x_i, y_j)$. In previous calculations the random on-site energies $V(\vec{x})$ were chosen to be uniformly distributed within a given energy interval $[-U/2, U/2]$ and each random sample from this distribution was drawn independently for each grid point. Since in this case the disorder value on each grid point has no correlation with the values on neighboring grid points we will refer to this type of disorder as “uncorrelated”. To go beyond this limitation and to account for the spatial correlations which naturally occur in realistic situations we choose our disorder potential such as to obey the Gaussian correlation function

$$C(\vec{r}) = \langle V(\vec{x}) \cdot V(\vec{x} + \vec{r}) \rangle \propto \exp\left(-\frac{r^2}{2\xi^2}\right) \quad (4)$$

where the brackets $\langle \dots \rangle$ stand for an average over all the grid points \vec{x} and many disorder realizations. The standard deviation of this Gaussian defines the correlation length ξ , which measures the spatial range of the correlations. The value of the disorder strength U is established by demanding

$$\begin{aligned} \langle V_{ij} \rangle &= 0, \\ \langle V_{ij}^2 \rangle &= \frac{U^2}{12}. \end{aligned} \quad (5)$$

These values are chosen such as to agree with those of the uncorrelated disorder potential distributed within the interval $[-U/2, U/2]$. See Fig. 1 for an illustration of the disorder potentials with and without spatial correlations in the employed tight-binding grid.

III. RESULTS

We first consider the conductance through a rectangular bar of a topological insulator (width $L_x = 2000 \text{ nm}$ and height $L_y = 500 \text{ nm}$) with topological mass $m = -10 \text{ meV}$. In the clean limit (see $U = 0$ in Fig. 2(a)) quantized edge transport (green area) only occurs in an energy range $|E_F| < |m|$.¹⁶ Adding now an *uncorrelated* disorder to the clean topological insulator extends this QSH phase and shifts its onset towards higher energies

(see $U > 0$ in Fig. 2(a) and Ref. [16]). This so-called TAI phase of quantized transport emerges in the presence of strong uncorrelated disorder and extends beyond the limits $|E_F| = |m|$. Our results from Fig. 2(a) agree very well with the literature,¹⁶ thereby confirming the validity of our simulations.

In a next step we repeat this calculation for a *correlated* disorder potential. We choose the value of the correlation length $\xi = 23.45$ nm considerably larger than the grid constant $a = 5$ nm but still much smaller than the height $L_y = 500$ nm of the sample. Our results for such a finite correlation length (see Fig. 2(b)) differ dramatically from the uncorrelated case (see Fig. 2(a)): Apparently the chosen spatial correlations in the disorder lead to a total breakdown of the TAI conductance plateau. We also observe an increased disorder-sensitivity as well as a narrowing of the conductance plateau corresponding to the original QSH phase in the clean limit. These results demonstrate that spatial correlations in the disorder add an important new component to the physics of topological insulators. Especially in view of the envisioned experiments that probe the physics of strongly disordered topological insulators, our results can apparently be expected to impose rather strict limits on the observability of the TAI phase. For such an experimental realization of the TAI we can certainly conclude that it is equally important to be able to control the correlation length ξ as it is to control the strength U of a disorder potential.

In a next step we performed additional calculations to check the influence of spatial correlations also for larger samples than the ones considered above. This is particularly important as finite-size effects in small samples due to a coupling of counter-propagating edge states can considerably distort the phase diagram of the TAI.^{27,28,43} To determine these phase boundaries in extended samples we performed a scaling analysis following previous work in this direction.^{19,45} For this purpose a quadratic geometry of size $L = L_x = L_y$ is rolled up to a cylinder^{17,27,45} using periodic boundary conditions in y -direction which eliminate the edge states in the sample. The disorder-averaged logarithmic conductance $\langle \ln G \rangle$ of the remaining bulk states is then calculated for three different sizes $L_1 < L_2 < L_3$ of the quadratic system. The crossing points of $\langle \ln G \rangle$ calculated for samples of different sizes determine the disorder boundaries at which the bulk states make transitions between different characteristic transport regimes.⁴⁵ We calculated these phase transition points for an uncorrelated and for correlated potentials with different correlation length ξ in systems of three different sizes $L_1 = 500$ nm, $L_2 = 700$ nm and $L_3 = 1050$ nm. Due to the high numerical effort involved, we restrict ourselves to a single energy of $E_F = 16$ meV at which the TAI conductance plateau in the uncorrelated case is wide and well established (see Fig. 2(a)).

The results of our scaling analysis are shown in Fig. 3: Considering first the uncorrelated case studied already earlier (see black curves) we find that the lowest cross-

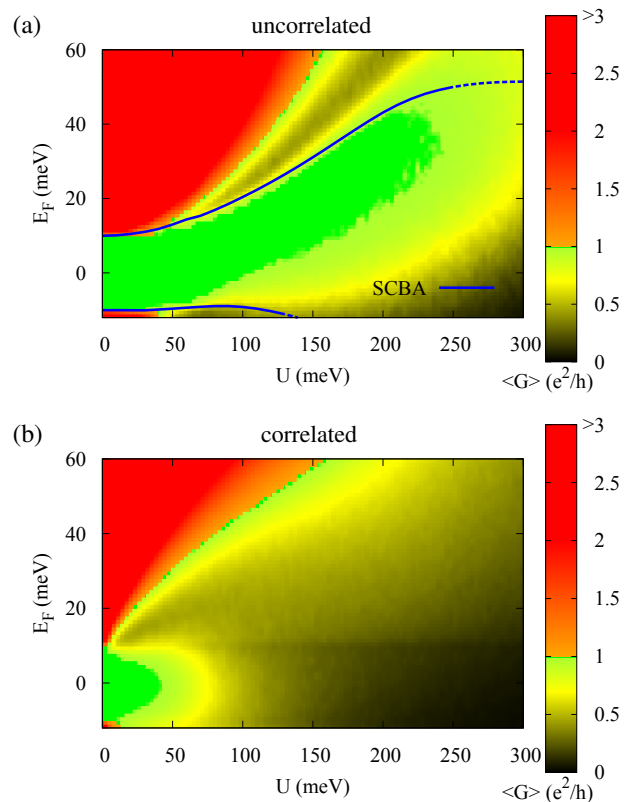


FIG. 2. (color online). Average conductance $\langle G \rangle$ as a function of disorder strength U and Fermi energy E_F through a topological insulator ($m = -10$ meV). The system length $L_x = 2000$ nm and the height $L_y = 500$ nm. The average is taken over (a) 200 and (b) 1000 disorder realizations. The green area shows where the average conductance $\langle G \rangle$ reaches a plateau at a single conductance quantum e^2/h originating from edge transport through the disordered system. (a) For uncorrelated disorder the TAI phase appears at energies $E_F > |m|$ and strong disorder. The blue lines show the phase boundaries of the TAI predicted by the effective medium theory which is based on the self-consistent Born approximation (SCBA) shown in Eq. (6). (b) Spatial correlations in the disorder with correlation length $\xi = 23.45$ nm destroy the TAI conductance plateau and narrow the plateau to an interval within the original bulk band gap.

ing point occurs at a value of the disorder strength $U \approx 70$ meV which fits well with the onset of the aforementioned TAI conductance plateau in Fig. 2(a) (see also Ref. [45]). This onset coincides here with the opening of a bulk band gap which is reflected in the scaling plots of Fig. 3 through a dramatic reduction of the conductance by more than ten orders of magnitude. The second and third crossing points, in turn, can be associated with the breakdown of the TAI phase observed in Fig. 2(a). The corresponding transition is, however, not induced by a band edge but rather by a mobility edge associated with those bulk states that fill the band gap when increasing the disorder strength beyond the first crossing point. These bulk states undergo a delocalization-localization

transition at the second and third crossing point which destroys the conductance plateau as soon as the delocalized bulk states start coupling the edge states at opposite edges in the sample. Note that for this to happen it is already sufficient for individual rather than for all bulk states to delocalize such that finite size effects do play a role at this strong-disorder boundary of the TAI.^{45,46}

When extending the above scaling analysis now to the case of correlated disorder with successively increasing correlation length ξ we find a behavior different from the uncorrelated case: already for the case of very short-range correlations with $\xi = 9.0$ nm (red curves in Fig. 3) significant differences appear. We still find three crossing points as before, but the conductance no longer displays the very strong suppression associated with a bulk band gap. Instead, we find that the delocalization-localization region of bulk states, which was previously associated with the strong-disorder boundary of the TAI, widens for increasing correlation length ξ . Correspondingly, in the disorder interval between the first and the second crossing points (which are now also much closer together) the conductance is much less suppressed than in the uncorrelated case. This indicates that in the correlated case the bulk band gap disappeared and was filled with localized bulk states. We emphasize, however, that both a band gap as well as localized bulk states can give rise to a TAI, as was explicitly pointed out in a recent study.⁴⁶ In what was termed a TAI-I phase the coupling between edge states is prevented by a bulk band gap which eliminates all bulk states that would mediate such a coupling. A second TAI-II phase was characterized by a coexistence of localized bulk-states and extended edge-states. As long as the localization length of these bulk states remains smaller than the width of the sample, the coupling of edge states remains suppressed and the TAI persists. Following these arguments, the transition into the TAI phase can either occur at a band edge (for TAI-I) or at a mobility edge (for TAI-II). From this we conclude that the original band edge at the weak-disorder boundary of the TAI-I phase in the uncorrelated case gets replaced by a mobility edge as the new weak-disorder boundary of a TAI-II phase in the correlated case. The corresponding suppression of the TAI-I phase already at a rather small correlation length of $\xi = 9.0$ nm suggests that the TAI-II phase is more robust to spatial disorder correlation than the TAI-I phase. The TAI-II phase is, in turn, more sensitive to finite size effects due to *individual* localized bulk states which can couple counter-propagating edge states. Correspondingly we can understand the absence of a TAI conductance plateau in Fig. 2(b) and Fig. 4 in between the first and second crossing points of our scaling analysis in Fig. 3 as a finite-size effect which may disappear for much larger samples than studied here. Further explicit calculations will also be necessary to better understand the infinite-size limit for TIs with long-range correlations in the disorder. Our own results for the case of $\xi = 35$ nm (see the blue curves in Fig. 3) show that the widening of the delocalization-localization transition

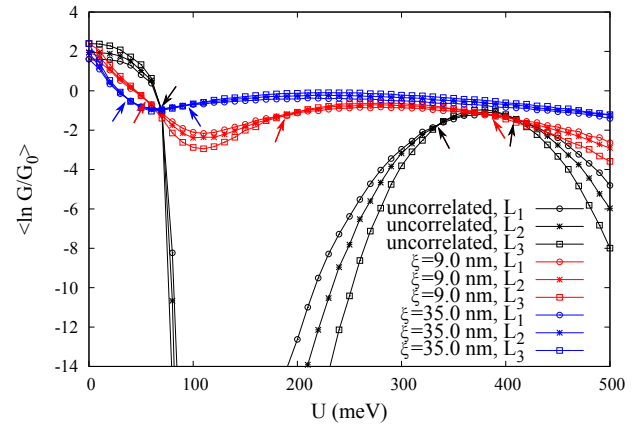


FIG. 3. (color online). Average logarithmic conductance $\langle \ln G \rangle$ as a function of disorder strength U for different system sizes $L_1 = 500$ nm, $L_2 = 700$ nm and $L_3 = 1050$ nm for uncorrelated disorder (black) and correlated disorder with correlation length $\xi = 9.0$ nm (red) and $\xi = 35.0$ nm (blue) at an energy of $E_F = 16$ meV (disorder average taken over 2000 configurations). The transitions into and out of the TAI phase can be seen by the crossing points of curves with equal color. In the correlated case the TAI bulk band gap between the first and second crossing point disappears and the delocalization-localization region between second and third crossing point is broadened.

continues for increasing correlation length ξ . However, since the transition region for $\xi = 35$ nm is here already very wide, detailed statements on the phase boundaries in the infinite size limit are difficult to deduce from our finite-size calculations.

While further calculations will thus be required to elucidate the infinite size limit of the TAI-II phase, we can further corroborate our arguments from above with respect to the suppression of the TAI-I phase due to correlations in the disorder. If these arguments are correct, the QSH phase (characterized by a negative topological mass and a chemical potential in the band gap, $|\mu| < |m|$) should border, in the correlated disorder case, directly on the surviving TAI-II phase (characterized by a negative topological mass and a chemical potential outside of the band gap, $|\mu| > |m|$). In the corresponding plot in Fig. 2(b) we see that the QSH conductance plateau (existing in the energy-range -10 meV $< \mu < 10$ meV in the disorder-free sample) extends only to much smaller values of disorder strength U than in the uncorrelated case (compare with Fig. 2(a)). Since for the above arguments the borders of this reduced QSH conductance plateau with the neighboring TAI-II phase are characterized by a band edge crossing, these borders should be describable in terms of a similar effective medium theory as has been developed for the uncorrelated case.¹⁷ This theory maps the disordered system onto a disorder-free sample with a renormalized topological mass $\bar{m} = m + \delta m$ and chemical potential $\bar{\mu} = \mu + \delta \mu$. This renormalization was carried out in terms of the self-consistent Born approximation

(SCBA) using an integral equation for the self-energy Σ :

$$\Sigma = \frac{U^2}{12} \left(\frac{a}{2\pi} \right)^2 \lim_{\kappa \rightarrow 0} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk_x dk_y \times \left(E_F + i\kappa - H_0(\vec{k}) - \Sigma \right)^{-1} . \quad (6)$$

Whenever the renormalized chemical potential reaches the edge of the band gap ($|\bar{\mu}| = |\bar{m}|$) the border of the QSH phase has been reached. Since this indicator, as calculated through the above SCBA, is independent of the system size, the effective medium theory offers an insightful and practical tool to determine the boundaries of the QSH phase in the infinite-size limit.

In order to generalize the effective medium theory from above to the case of spatially correlated potentials we resort to recent theoretical work in which an extension of the coherent potential approximation to correlated disorder was proposed.⁵⁰ Following this line of work, one can conveniently include the disorder correlations through an additional term in Eq. (6) which is given by the normalized Fourier transform of the disorder correlation function,⁵¹ $\tilde{C}(\vec{k})$,

$$\Sigma = \frac{U^2}{12} \lim_{\kappa \rightarrow 0} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk_x dk_y \tilde{C}(\vec{k}) \times \left(E_F + i\kappa - H_0(\vec{k}) - \Sigma \right)^{-1} . \quad (7)$$

Since in the present case of Gaussian disorder correlations [see Eq. (4)] the expression for $\tilde{C}(\vec{k})$ is a Gaussian itself (centered around $k = 0$), the effect of the disorder correlations is to smoothly cut off the above integral. The more long-range the correlations are (in real space), the sharper this cut-off is (in Fourier space).

To extract the corrections δm and $\delta \mu$ from the self-energy in Eq. (7), we proceed along the lines of the uncorrelated case¹⁷ and decompose the self-energy into the Pauli matrices σ_i

$$\Sigma = \Sigma_0 \sigma_0 + \Sigma_x \sigma_x + \Sigma_y \sigma_y + \Sigma_z \sigma_z \quad (8)$$

with the help of

$$\begin{aligned} \delta m &= \text{Re } \Sigma_z , \\ \delta \mu &= -\text{Re } \Sigma_0 . \end{aligned} \quad (9)$$

With the values extracted for the renormalized topological mass $\bar{m} = m + \delta m$ and chemical potential $\bar{\mu} = E_F + \delta \mu$, we can now estimate the boundaries of the QSH phase in the case of correlated disorder by determining the values of E_F and U for which the renormalized chemical potential $\bar{\mu}$ drops into the effective band gap at $\bar{\mu} = \pm \bar{m}$. We start by first testing our approach for the *uncorrelated* case, for which the weak disorder boundary of the TAI phase was estimated before. In this case the discrete Fourier transform of the correlation function $\tilde{C}(\vec{k})$ is constant. By normalizing this function in k -space

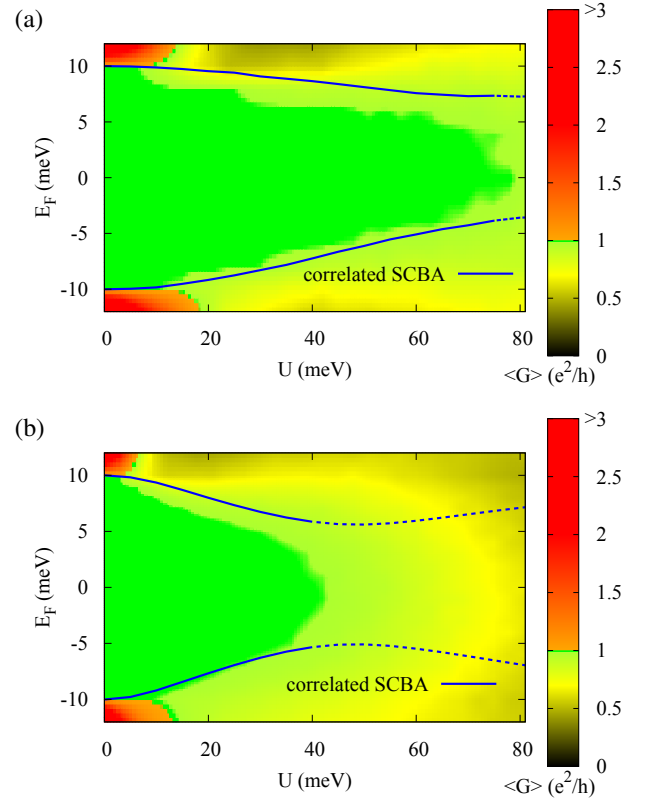


FIG. 4. (color online). The average conductance $\langle G \rangle$ as a function of Fermi energy E_F and disorder strength U is shown for the correlated case with correlation length (a) $\xi = 9$ nm and (b) $\xi = 23.45$ nm. The system is $L_x = 2000$ nm long and $L_y = 500$ nm high while the grid spacing $a = 5$ nm. The blue curves demonstrate the validity of our adapted effective medium theory from Eq. (7).

to the volume $V = (2\pi)^2/a^2$ of the Brillouin zone, we exactly reobtain the expression for the self energy in the uncorrelated case, Eq. (6). If we determine with this approach the phase boundaries of the QSH phase in the *uncorrelated* case we obtain the blue curves in Fig. 2(a) which fit nicely to the conductance plateau of the QSH and TAI phases and to previous calculations.^{16,17,45} Extending our calculations to the case of *correlated* disorder, the borders which we calculate through Eqs. (7) and (9) (see blue curves in Fig. 4) describe the boundaries of the QSH conductance plateau very well (without any adjustable parameters). The good agreement which we find for different correlation lengths ξ (see Fig. 4 parts (a) and (b)) corroborates the validity of our approach. Note that, in contrast to the uncorrelated case, no conductance plateau is observed for $|\mu| > |m|$ (i.e., outside of the energy region where the QSH phase is present in the clean sample). An increasing disorder strength rather leads to a narrowing of the bulk band gap within which pure QSH edge transport can occur. This reduced band gap corresponds to positive corrections δm and $\delta \mu$ in the case of a correlated potential whereas in the uncorre-

lated case these corrections were shown to be negative.¹⁷ It is exactly these positive corrections which lead to the breakdown of the TAI-I phase for $|\mu| > |m|$.

IV. CONCLUSION

In this work we investigate the effect of spatially correlated disorder on a two-dimensional topological insulator. We thereby extend previous studies in which only uncorrelated disorder potentials were considered.^{16,17,45,46} Our calculations show that a finite correlation of the disorder potential enhances finite-size effects and may entirely suppress a regime of quantized conductance known as the TAI phase. Such a suppression of the TAI phase has also been found for off-diagonal bond disorder originating from the deformation of the lattice.²² To describe the shifted boundaries of quantized conductance theoretically, we perform a scaling analysis and adapt an existing

effective medium theory to the case of spatially correlated potentials which yields quantitative agreement with our numerics. Our results suggest that for observing the TAI phase experimentally, it will be necessary to work with comparatively large samples (to suppress finite size effects) and with very short ranged disorder potentials as any long-range correlations may strongly suppress this topologically non-trivial phase. We speculate that spatial correlations might also be an important impediment to eliminate the bulk conductance in *three-dimensional* topological insulators.⁵² This would certainly constitute an interesting topic for further investigations.

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